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3.2 2.2

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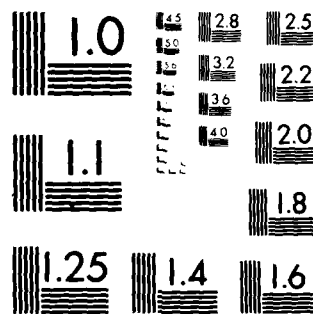
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Smoothing Splines: Regression, Derivatives
and Deconvolution

John Rice and Murray Rosenblatt

University of California, San Diego
La Jolla, California 92093

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Summary

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The statistical properties of a cubic smoothing spline and its derivative are analyzed. It is shown that unless unnatural boundary conditions hold, the integrated squared bias is dominated by local effects near the boundary. Similar effects are shown to occur in the regularized solution of a translation-kernel integral equation. These results are derived by developing a Fourier representation for a smoothing spline.

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1. Introduction and Summary

We consider statistical properties of smoothing splines and related procedures. Given $x_i = f(t_i) + \epsilon_i$, $i = 1,\ldots,n$ where g is an unknown smooth function and the ϵ_i are random errors, a cubic smoothing spline $g(t;\lambda)$ is the function which minimizes

$$\frac{1}{n} \sum_{i=1}^{n} [x_i - g(t_i)]^2 + \lambda \int (g''(t))^2 \, dt \; . \qquad (1.1)$$

Smoothing splines were proposed by Whittaker (1923), Schoenberg (1964), and Reinsch (1967). Some analysis of their statistical properties in the case that g and f are periodic appears in Wahba (1975) and Rice and Rosenblatt (1981). The method of cross validation for choosing the smoothing parameter λ from the data has been discussed in Craven and Wahba (1979).

Smoothing splines may be viewed in a larger context. Given $x_i = (Af)(t_i) + \epsilon_i$ where A is a linear operator, a "regularized" estimate of f is the function g which minimizes

$$\frac{1}{n} \sum_{i=1}^{n} [x_i - (Ag)(t_i)]^2 + \lambda \int (g''(t))^2 \, dt \; . \qquad (1.2)$$

Frequently Af is of the form

$$(Af)(t) = \int k(t,s) f(s) ds \; . \qquad (1.3)$$

Many examples of this type may be found in Tikhonov and Arsenin (1977). The method of regularization is used to control the instability that would arise if one tried to invert A or $A*A$. The regularized solutions have a formal resemblance to ridge-regression estimates; in both cases the variance

of the estimate is reduced at the cost of increasing bias. Although there is a large literature on this topic, there has been relatively little analysis of the statistical properties of the solutions.

In this paper we examine two cases of (1.3), numerical differentiation

$$(Af)(t) = \int_0^t f(u)du \tag{1.4}$$

and deconvolution,

$$(Af)(t) = \int_0^1 w(t-s)f(s)ds . \tag{1.5}$$

We next summarize and discuss our main results. Derivations and some further results are contained in later sections. We first deal with a cubic smoothing spline.

Consider observations

$$x_k = f(k/n) + \epsilon_k, \qquad k = 0,1,\ldots,n$$

with f continuously differentiable, $f'' \in L^2$ and the ϵ_k random variables with

$$E \epsilon_k \equiv 0$$

$$E \epsilon_k \epsilon_j = \delta_{k,j} \sigma^2, \qquad \sigma^2 > 0 .$$

We wish to determine a continuously differentiable function $g = g(t;\lambda,n)$ with $g'' \in L^2$ that minimizes

$$\frac{1}{n}\left\{\frac{1}{4}\left(x_0+x_n-g(0)-g(1)\right)^2 + \sum_{k=1}^{n-1}\left(x_k-g(k/n)\right)^2\right\}$$

$$+ \lambda \int_0^1 \left(g''(t)\right)^2 dt . \tag{1.6}$$

Here $\lambda = \lambda(n) > 0$ and the object is to determine $\lambda(n)$ as a function of n so that

$$\int_0^1 E[g(t)-f(t)]^2 dt$$

tends to zero as $n \to \infty$ at a rapid rate. The term

$$\frac{1}{2}\left(x_0+x_n\right) - \frac{1}{2}\left(g(0)+g(1)\right)$$

appears in (1.6) because one wishes to allow for the possibility that $f(0) \neq f(1)$ and in that case the Fourier series of $f(t)$ will converge to $\frac{1}{2}\left(f(0)+f(1)\right)$ at $t = 0,1$.

Theorem 1. *Let* $f \in C^2$. *If* $\lambda^3(n)n^8 \to \infty$, $\lambda(n) \to 0$ *as* $n \to \infty$ *then*

$$\int \sigma^2[g(t)]dt \cong \frac{\sigma^2\lambda^{-1/4}}{n} \, 3 \cdot 2^{-7/2} .$$

Theorem 2. *Let* $f \in C^4$. *Assume that* $\lambda^3(n)n^8 \to \infty$, $\lambda(n) \to 0$ *as* $n \to \infty$. *Then if* $f^{(2)}(0)$ *or* $f^{(2)}(1) \neq 0$

$$\int [E \, g(t)-f(t)]^2 \, dt \cong \{(f^{(2)}(0))^2 + (f^{(2)}(1))^2\} \, \lambda^{5/4} \, 2^{-3/2}$$

while if $f^{(2)}(0) = f^{(2)}(1) = 0$ *but* $f^{(3)}(0) \neq 0$ *or* $f^{(3)}(1) \neq 0$ *we have*

$$\int [E\ g(t)-f(t)]^2\ dt \cong \{(f^{(3)}(0))^2 + (f^{(3)}(1))^2\}$$

$$\lambda^{7/4}\ 3 \cdot 2^{-3/2}\ .$$

A common reason for nonparametric data smoothing is to calculate an extimate of the derivative of a function. Schemes for numerically differentiating noisy data that are closely related to the derivative of a smoothing spline have been proposed in Cullum (1971) and Anderssen and Bloomfield (1974). The properties of the derivative of a smoothing spline follow fairly directly from the properties of the smoothing spline itself.

Theorem 3. *If* $f \in C^2$ *and if* $\lambda n^5 \to \infty$ *as* $n \to \infty$ *and* $\lambda \to 0$, *then*

$$\int_0^1 \ ^2(g'(t))dt = \frac{\sigma^2}{n}\ \lambda^{-3/4} \cdot 2^{-7/2} + o(n^{-1}\lambda^{-3/2})\ .$$

Theorem 4. *Assume that* $f \in C^4$, *and that* $\lambda n^5 \to \infty$. *Then if* $f^{(2)}(0) \neq 0$ *or* $f^{(2)} \neq 0$

$$\int_0^1 [E\ g'(t)-f'(t)]^2\ dt \cong [(f^{(2)}(0))^2 + (f^{(2)}(1))^2] \cdot \lambda^{3/4} \cdot 3 \cdot 2^{-3/2}\ :$$

If $f^{(2)}(0) = f^{(2)}(1) = 0$, *but* $f^{(3)}(0)$ *or* $f^{(3)}(1) \neq 0$ *then*

$$\int_0^1 [E\ g'(t)-f'(t)]^2\ dt \cong [(f^{(3)}(0))^2 + (f^{(3)}(1))^2]\lambda^{5/4} \cdot 3 \cdot 2^{-3/2}\ .$$

Comparing these results to Theorems 1 and 2 we see that the variance and integrated squared bias of the derivative are a factor of $\lambda^{-1/2}$ larger than the variance and integrate square bias of the function itself.

Theorem 2 shows that the integrated squared bias is dominated by contributions from the boundary unless g satisfies the condition $g^{(k)}(0) = g^{(k)}(1) = 0, k = 2,3$. Lemma 6 of section 3 gives a local approximation to the bias in the case that these conditions are not met. Roughly, the bias decays like $\exp(-2^{-1/2}\lambda^{-1/4}t)$ trigonometrically modulated. In the interior of $[0,1]$ the squared bias is proportional to λ^2.

These results are not unexpected. The smoothing spline is a "natural" spline and satisfies the two arbitrary end conditions $f''(0) = f''(1) = 0$. In the context of pure interpolation the use of a natural spline is usually not recommended since the error near the ends is of order h^2 where h is the mesh size whereas other methods can produce an error uniformly of order h^4, if $f \in C^4$, de Boor (1978), Powell (1981). Similarly, it can be shown that the boundary effect dominates the integrated squared error, Rosenblatt (1976). In the nonstochastic framework methods of estimating the boundary constraints have been proposed in these references and it would appear plausible that a similar approach might work in the stochastic case.

Natural splines in the nonstochastic setting and smoothing splines in the stochastic setting are the optimal solutions of certain minimax problems, Powell (1981) and Speckman (1981). It appears that flexibility is lost by guarding against worst cases.

Smoothing splines have also been proposed in the case of spectral density estimation (see Cogburn and Davis (1974) and Wahba (1980)). Boundary effects similar to those studied here occur in the case of periodic smoothing splines unless the function is smoothly periodic (see Rice and Rosenblatt (1980)).

The aliasing in the case of spectral analysis of discretely sampled data implies that boundary behavior will not be smooth in this context.

In the deconvolution problem we consider observations

$$x_k = F(k/n) + \varepsilon_k, \qquad k = 0,\ldots,n$$

where $F(k/n) = \int_0^1 w(k/n-u)f(u)du$, with $f^\sim \in L^2$ and the ε_k uncorrelated random variables with mean 0 and variance σ^2. The regularized approximation to f is the function g that minimizes

$$\frac{1}{4n}(x_0+x_n-G(0)-G(1))^2 + \frac{1}{n}\sum_{k=1}^{n-1}(x_k-G(k/n))^2$$

$$+ \lambda \int_0^1 (g^\sim(t))^2\, dt \; . \tag{1.7}$$

Here $G(k/n) = \int_0^1 w(k/n-u)f(u)du$. The kernel of the integral equation, w, is the periodic extension of a function defined on $[0,1]$, and it is assumed that $w \in L^2$. We assume that the Fourier coefficients w_k of w are nonzero for all k.

The constants that occur in the asymptotic expressions for the components of the integrated mean square error depend on the exact form of w, but the rates of decrease depend only on the rate of decrease of the Fourier coefficients w_k of w. Paralleling Theorems 1 and 2 we have

<u>Theorem 5.</u> *Let* $f \in C^2$ *and suppose that* $|w_k|^2 \sim k^{-2\beta}$, $\beta > 0$. *If* $\lambda n^{2\beta+3} \to \infty$

$$\int \sigma^2[g(t)]dt \sim n^{-1} \lambda^{-(2\beta+1)/(2\beta+4)} .$$

Theorem 6. *Let* $f \in C^4$ *and suppose that* $|w_k|^2 \sim k^{-2\beta}$, $\beta > 0$ *and* $\lambda n^{2\beta+3} \to \infty$ *as* $n \to \infty$. *Then if* $f''(0)$ *or* $f''(1) \neq 0$

$$\int [E \, g(t) - f(t)]^2 \, dt \sim \lambda^{5/(2\beta+4)} .$$

If $f''(0) = f''(1) = 0$ *but* $f^{(3)}(0)$ *or* $f^{(3)}(1) \neq 0$, *then*

$$\int [E \, g(t) - f(t)]^2 \, dt \sim \lambda^{7/(2\beta+4)} .$$

If $f^{(k)}(0) = f^{(k)}(1)$, $k = 2,3$ *then*

$$\int [E \, g(t) - f(t)]^2 \, dt \sim \lambda^{8/(2\beta+4)} .$$

Analytic expressions for the approximate local bias are not available, but the qualitative behavior is similar to that of a smoothing spline.

Note that if w is very smooth, β is large, and the integrated mean square error will tend to zero relatively slowly.

2. Examples

The function $f(t) = \cos(2\pi t) + 4\cos(\pi t)$ satisfies $f''(0) = -8\pi^2$, $f''(1) = 0$, $f'''(0) = f'''(1) = 0$. Figures 1 and 2 show the exact bias of the smoothing spline estimate of the function and its derivative for 50 equi-spaced sampling points and $\lambda = 10^{-6}$. The effect of $f''(0)$ is clearly evident. The asymptotic analysis (Lemma 6) predicts that the bias,

$$b(t) \cong f''(0)\lambda^{1/2} \exp(-t\, 2^{-1/2}\lambda^{-1/4})$$

$$\cdot [\sin(t\, 2^{-1/2}\lambda^{-1/4}) - \cos(t\, 2^{-1/2}\lambda^{-1/4})] .$$

From this expression we see that the first zero-crossing of the bias should occur at $t = \pi\lambda^{1/4}\, 2^{-3/2} = .035$ and that $b'(t)$ should be zero at $t = \pi\lambda^{1/4}\, 2^{-1/2} = .070$, which is borne out in Figure 1. Figure 2 shows that the bias of the derivative is larger by a factor of about $\lambda^{-1/4}$.

We next consider the deconvolution problem wherein f is convolved with a function w, the graph of which is an isosceles triangle centered at 0 with height 20 and base .4. This is intended to correspond to a situation in which averaged values of f are measured with error. Since the analysis of section 4 requires that w be periodically extended, the triangle is also centered over -1 and 1. To calculate the bias, (1.7) was discretized assuming 25 equi-spaced observations and the solution was computed at 50 equi-spaced points. Other mesh sizes were tried to insure that the results did not merely reflect the discretization. The calculations were done on a VAX 11/80 in double precision. Figure 3 shows the bias for $\lambda = 10^{-8}$; there is a clear effect near 0 and also an effect near 1. The shapes are qualitatively similar to Figure 1.

Since the assumption that w is periodically extended is clearly somewhat artificial, we also computed the bias for w just corresponding to a triangle centered over 0. The resulting bias is shown in Figure 4. Here the only effect is near 0; the effect near 1 of Figure 3 is apparently due to the periodicity of w.

3. The Smoothing Spline and Its Derivative

In this section we derive Theorems 1-4 and some auxiliary results.
In order to do this we carry out a Fourier analysis of the smoothing spline.

Notice that

$$g_k = \int_0^1 e^{2\pi i k t} g(t) dt = \Delta g^0 a_k - \Delta g^1 b_k + h_k b_k \tag{3.1}$$

for $k \neq 0$ where

$$\Delta g^0 = g(1) - g(0)$$

$$\Delta g^1 = g'(1) - g'(0)$$

$$h_k = \int_0^1 e^{2\pi i k t} g'(t) dt .$$

Let

$$y_j = \begin{cases} \frac{1}{2} (x_0 + x_n) & \text{if} \quad j = 0 \\ x_j & \text{if} \quad j = 1, \ldots, n-1 \end{cases}$$

and set

$$\hat{y}_j = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} y_j \exp (2\pi i j k / n) .$$

Given a sequence of coefficients p_k we will let $p_k^{(n)}$ denote the corresponding set of aliased coefficients arising in a discrete Fourier analysis

$$p_k^{(n)} = \sum_{s=-\infty}^{\infty} p_{k+sn}, \qquad k = 0,1,\ldots,n-1 \ .$$

Also let

$$\tilde{p}_0^{(n)} = p_0^{(n)} - p_0 = \sum_{s \neq 0} p_{sn}$$

and

$$\hat{z}_k = \frac{\hat{y}_k}{\sqrt{n}} - \Delta g^0 a_k^{(n)} + \Delta g^1 b_k^{(n)}, \qquad k = 1,\ldots,n-1 \ . \tag{3.2}$$

<u>Lemma 1</u>. *Let* f *and* Δg^0, Δg^1 *be given. Assume that* f,g *are continuously differentiable with* $f^{\sim}, g^{\sim} \in L^2$. *Then the function* g *minimizing* (1.1) *is determined by the following specification on Fourier coefficients:*

$$g_0 = \frac{\hat{y}_0}{\sqrt{n}} - \Delta g^0 \tilde{a}_0^{(n)} + \Delta g^1 b_0^{(n)} \ , \tag{3.3}$$

$$h_{sn} = 0 \quad \text{for} \quad s \neq 0 \ , \tag{3.4}$$

$$h_{k+sn} = \frac{1}{\lambda + r_k} b_{k+sn} \ \hat{z}_k \tag{3.5}$$

for $k = 1,\ldots,n-1$ *and integral* s. *Here it is understood that*

$$r_k = \sum_s (2\pi(k+sn))^4 \ .$$

The Parseval relation implies that (1.1) can be rewritten as

$$\left|\frac{\hat{y}_0}{\sqrt{n}} - g_0 - \tilde{g}_0^{(n)}\right|^2 + \sum_{k=1}^{n-1} \left|\frac{\hat{y}_k}{\sqrt{n}} - \Delta g^0 a_k^{(n)} + \Delta g^1 b_k^{(n)} - (h_k b_k)^{(n)}\right|^2$$

$$+ \lambda\left[(\Delta g^1)^2 + \sum_{k\neq 0}\sum_s |h_{k+sn}|^2 + \sum_{s\neq 0} |h_{sn}|^2\right] . \tag{3.6}$$

In minimizing this expression, one can separately minimize the sum of the terms with k fixed for each value of k. Minimizing for $k = 0$ leads one to (3.3) and (3.4). For $k \neq 0$ we have

$$\lambda h_{k+sn} = (\hat{z}_k - (h_k b_k)^{(n)})b_{k+sn} . \tag{3.7}$$

Multiplying by b_{k+sn} and summing over s leads to

$$(h_k b_k)^{(n)} = \frac{\hat{z}_k r_k}{\lambda + r_k} \tag{3.8}$$

and this together with (3.7) leads to (3.5).

<u>Lemma 2</u>. *Insert (3.3), (3.4) and (3.5) in (3.6). Minimizing the resulting expression with respect to* Δg^0, Δg^1 *leads to*

$$\Delta g^0 = \left\{\sum_{k=1}^{n-1} \frac{\hat{y}_k}{\sqrt{n}} \overline{a_k^{(n)}} \Big/ (\lambda + r_k)\right\}\left\{\sum_{k=1}^{n-1} |a_k^{(n)}|^2/(\lambda + r_k)\right\}^{-1} \tag{3.9}$$

and

$$\Delta g^1 = -\left\{\sum_{k=1}^{n-1} \frac{\hat{y}_k}{\sqrt{n}} b_k^{(n)} \Big/ (+ r_k)\right\}\left\{1 + \sum_{k=1}^{n-1} |b_k^{(n)}|^2/(\lambda + r_k)\right\}^{-1} . \tag{3.10}$$

If we insert (3.3), (3.4) and (3.5) in the expression (3.7), the result can be written as

$$\lambda |\Delta g^1|^2 + \lambda \sum_{k=1}^{n-1} \frac{|\hat{z}_k|^2}{\lambda + r_k} . \tag{3.11}$$

Minimizing this expression with respect to Δg^0 and Δg^1 leads to the following equations

$$\sum_{k=1}^{n-1} \frac{\hat{z}_k \bar{a}_k^{(n)}}{\lambda + r_k} = 0 \tag{3.12}$$

$$\Delta g^1 + \sum_{k=1}^{n-1} \frac{\hat{z}_k b_k^{(n)}}{\lambda + r_k} = 0 . \tag{3.13}$$

On solving for Δg^0, Δg^1 the expressions (3.7) and (3.10) are obtained.

<u>Lemma 3</u>. *The function* g *minimizing* (1.1) *has Fourier coefficients*

$$g_0 = \frac{\hat{y}_0}{\sqrt{n}} + \Delta g^1 \bar{b}_0^{(n)} \tag{3.14}$$

$$g_{sn} = \Delta g^0 a_{sn} - \Delta g^1 b_{sn} \quad \text{for} \quad s \neq 0 \tag{3.15}$$

and for $k = 1, \ldots, n-1$ *and* s *integral*

$$g_{k+sn} = \Delta g^0 [a_{k+sn} - \frac{1}{\lambda + r_k} |b_{k+sn}|^2 a_k^{(n)}]$$

$$- \Delta g^1 [b_{k+sn} - \frac{1}{\lambda + r_k} |b_{k+sn}|^2 b_k^{(n)}]$$

$$+ \frac{|b_{k+sn}|^2}{\lambda + r_k} \frac{\hat{y}_k}{\sqrt{n}} \tag{3.16}$$

with Δg^0, Δg^1 *given by* (3.9) *and* (3.10).

The fact that $\tilde{a}_0^{(n)} = 0$ and (3.3) holds lead to (3.14). Also (3.4) and (3.5) inserted in (3.1) yield (3.15) and (3.16).

The integrated mean square error of $g(t)$ as a function of $f(t)$ is

$$\int_0^1 E[g(t)-f(t)]^2 \, dt$$

$$= \int_0^1 \text{var}(g(t))dt + \int_0^1 [E\, g(t)-f(t)]^2 \, dt \; . \qquad (3.17)$$

Moreover

$$\int_0^1 \text{var}(g(t))dt = \text{var}(g_0) + 2 \sum_{k=1}^{\infty} \text{var}(g_k) \; . \qquad (3.18)$$

It should be noted that the g_k's are complex-valued random variables. The covariance of two complex-valued random variables U,V is understood to be

$$\text{cov}(U,V) = E\{(U-EU)\overline{(V-EV)}\} \; .$$

We shall now derive Theorem 1. Notice that Δg^0 and Δg^1 are real even though they are written in complex form. It is clear that

$$\text{cov}(\hat{y}_j,\hat{y}_k) = \left(\delta_{j,k} - \frac{1}{2n}\right)\sigma^2 \qquad (3.19)$$

for $j,k = 0,1,\ldots,n-1$. From (3.19) it follows that

$$\sigma^2(\Delta g^0) \cong \frac{\sigma^2}{n} \left\{ \sum_{k=1}^{n-1} |a_k^{(n)}|^2 \Big/ (\lambda+r_k)^2 \right\}$$
$$\left\{ \sum_{k=1}^{n-1} |a_k^{(n)}|^2 \Big/ (\lambda+r_k) \right\}^{-2} \tag{3.20}$$

$$\sigma^2(\Delta g^1) \cong \frac{\sigma^2}{n} \left\{ \sum_{k=1}^{n-1} |b_k^{(n)}|^2 \Big/ (\lambda+r_k)^2 \right\}$$
$$\left\{ 1 + \sum_{k=1}^{n-1} |b_k^{(n)}|^2 \Big/ (\lambda+r_k) \right\}^{-2} . \tag{3.21}$$

Since

$$\sum_{k=1}^{n-1} |a_k^{(n)}|^2 \Big/ (\lambda+r_k) \cong \sum_{|k|\leq\frac{n}{2}} |2\pi k|^2 \Big/ (\lambda|2\pi k|^4+1)$$
$$\cong \lambda^{-3/4} C_1 , \tag{3.22}$$

$$\sum_{k=1}^{n-1} |a_k^{(n)}|^2 \Big/ (\lambda+r_k)^2 \cong \lambda^{-7/4} C_2 , \tag{3.23}$$

$$\sum_{k=1}^{n-1} |b_k^{(n)}|^2 \Big/ (\lambda+r_k) \cong \lambda^{-1/4} C_3 , \tag{3.24}$$

$$\sum_{k=1}^{n-1} |b_k^{(n)}|^2 \Big/ (\lambda+r_k)^2 \cong \lambda^{-5/4} C_4 , \tag{3.25}$$

where

$$C_1 = \int \frac{|2\pi x|^2}{|2\pi x|^4+1} dx , \qquad C_2 = \int \frac{|2\pi x|^6}{(|2\pi x|^4+1)^2} dx ,$$

$$C_3 = \int \frac{dx}{|2\pi x|^4+1} , \qquad C_4 = \int \frac{|2\pi x|^4}{(|2\pi x|^4+1)^2} dx$$

if $\lambda(n)n^4 \to \infty$ as $n \to \infty$, it can be seen that

$$\sigma^2(\Delta g^0) \cong \frac{\sigma^2}{n} C_2 C_1^{-2} \lambda^{-1/4} , \tag{3.26}$$

$$\sigma^2(\Delta g^1) \cong \frac{\sigma^2}{n} C_4 C_3^{-2} \lambda^{-3/4} , \tag{3.27}$$

if $\lambda(n)n^4 \to \infty$ as $n \to \infty$. The term

$$\sum_s \sum_{k=1}^{n-1} |a_{k+sn} - \frac{1}{\lambda + r_k} |b_{k+sn}|^2 a_k^{(n)}|^2 \tag{3.28}$$

occurs as a coefficient of $\sigma^2(\Delta g^0)$ in contributing to (3.18). However, (3.28) can be approximated by

$$\lambda^2 \sum_k \frac{|2\pi i k|^6}{(\lambda |2\pi k|^4 + 1)^2} \cong \lambda^{1/4} C_2 \tag{3.29}$$

with an error $O\left(\frac{1}{n}\right)$ if $\lambda(n)n^4 \to \infty$ as $n \to \infty$. The term

$$\sum_s \sum_{k=1}^{n-1} |b_{k+sn} - \frac{1}{\lambda + r_k} |b_{k+sn}|^2 b_k^{(n)}|^2 \tag{3.30}$$

arises as a coefficient of $\sigma^2(\Delta g^1)$ in contributing to (3.18). An estimation procedure similar to that used in arriving at (3.39) shows that (3.30) can be approximated by

$$\lambda^2 \sum_k \frac{|2\pi i k|^4}{(\lambda |2\pi k|^4 + 1)^2} \cong \lambda^{3/4} C_4 \tag{3.31}$$

with an error $O\left(\dfrac{1}{n^2}\right)$ if $\lambda^3(n)n^8 \to \infty$ as $n \to \infty$. The estimates obtained for (3.28) and (3.30) imply that the contribution to (3.18) from the terms involving Δg^0 and Δg^1 in (3.16) is

$$O\left(\frac{1}{n}\right)$$

if $\lambda^3(n)n^8 \to \infty$ as $n \to \infty$. Now consider the contribution from the last term on the right of (3.16). We shall see that it makes the major contribution to the integrated variance. The expression

$$\sum_s \sum_{k=1}^{n-1} \frac{|b_{k+sn}|^4}{|\lambda+r_k|^2} \frac{1}{n} \tag{3.32}$$

can be approximated by

$$\sum_{0<|k|<\frac{n}{2}} \frac{1}{\left(|2\pi k|^4+1\right)^2} \frac{1}{n} \cong \frac{\lambda^{-1/4}}{n} C_5 \tag{3.33}$$

where

$$C_5 = \int \frac{dx}{\left(|2\pi x|^4+1\right)^2}$$

with an error $O\left(\dfrac{1}{n}\right)$ if $\lambda(n)n^3 \to \infty$ as $n \to \infty$. Theorem 1 follows from these estimates.

Our next object is to derive Theorem 2 for the integrated squared bias of g as an estimate of f. Notice that for $k \neq 0$ we have

$$f_k = \int_0^1 e^{2\pi i k t} f(t) dt = \Delta f^0 a_k - \Delta f^1 b_k + m_k b_k \qquad (3.34)$$

with

$$m_k = \int_0^1 e^{2\pi i k t} f'(t) dt . \qquad (3.35)$$

Using (3.34) it is clear that

$$\frac{1}{2}(f(0)+f(1)) = \sum_{k=-\infty}^{\infty} f_k = \sum_{k=0}^{n-1} f_k^{(n)} ,$$

$$\iota(j/n) = \sum_{j=-\infty}^{\infty} f_k \exp(-2\pi i j k/n) \qquad (3.36)$$

$$= \sum_{k=0}^{n-1} f_k^{(n)} \exp(-2\pi i j k/n), \quad j = 1,\ldots,n-1 .$$

This implies that

$$E \, \hat{y}_j / \sqrt{n} = f_j^{(n)}, \qquad j = 0,1,\ldots,n-1 . \qquad (3.37)$$

From (3.34) it follows that

$$f_j^{(n)} = \Delta f^0 a_j^{(n)} - \Delta f^1 b_j^{(n)} + (m_j b_j)^{(n)}, \quad j = 1,\ldots,n-1 .$$

Relations (3.9), (3.10), and (3.37) imply that

$$E \Delta g^0 = \Delta f^0 + \left\{ \sum_{k=1}^{n-1} (m_k b_k)^{(n)} \overline{a}_k^{(n)} \Big/ (\lambda + r_k) \right\}$$

$$\left\{ \sum_{k=1}^{n-1} |a_k^{(n)}|^2 \Big/ (\lambda + r_k) \right\}^{-1} \tag{3.38}$$

and

$$E \Delta g^1 = \Delta f^1 \left[1 - \left\{ 1 + \sum_{k=1}^{n-1} |b_k^{(n)}|^2 \Big/ (\lambda + r_k) \right\}^{-1} \right]$$

$$- \left\{ \sum_{k=1}^{n-1} (m_k b_k)^{(n)} b_k^{(n)} \Big/ (\lambda + r_k) \right\}$$

$$\left\{ 1 + \sum_{k=1}^{n-1} |b_k^{(n)}|^2 \Big/ (\lambda + r_k) \right\}^{-1} . \tag{3.39}$$

Since we are dealing with real-valued functions f it follows that

$$m_k = \overline{m}_{-k}$$

and

$$(m_k b_k)^{(n)} = (\overline{m_{-k} b_{-k}})^{(n)} .$$

These last two relations together with (3.38) and (3.39) imply that

$$E \Delta g^0 - \Delta f^0 \cong - \left\{ \sum_{k=-\infty}^{\infty} \frac{(2\pi k) \operatorname{Im} m_k}{1 + \lambda |2\pi k|^4} \right\} \left\{ \sum_{k=-\infty}^{\infty} \frac{(2\pi k)^2}{1 + \lambda |2\pi k|^4} \right\}^{-1} \tag{3.40}$$

and

$$E \ \Delta g^1 - \Delta f^1 \cong - \left\{ \sum_{k=-\infty}^{\infty} \frac{\text{Re } m_k}{1+\lambda |2\pi k|^4} \right\} \left\{ \sum_{k=-\infty}^{\infty} \frac{1}{1+\lambda |2\pi k|^4} \right\}^{-1} . \tag{3.41}$$

If $f \in C^3$ one can see that

$$\text{Re } m_k = \int_0^1 f''(x) \cos 2\pi kx \ dx$$

$$= \int_0^1 \frac{1}{2} \{f''(x) + f''(-x)\} \cos 2\pi kx \ dx \tag{3.42}$$

and

$$2\pi k \ \text{Im } m_k = 2\pi k \int_0^1 f''(x) \sin 2\pi kx \ dx$$

$$= - \Delta f^2 + \int_0^1 f^{(3)}(x) \cos 2\pi kx \ dx$$

$$= - \Delta f^2 + \int_0^1 \frac{1}{2} \{f^{(3)}(x) + f^{(3)}(-x)\} \cos 2\pi kx \ dx \tag{3.43}$$

with

$$\Delta f^2 = f^{(2)}(1) - f^{(2)}(0) .$$

From (3.16) it follows that for $k = 1, \ldots, n-1$

$$E \ g_{k+sn} - f_{k+sn} = (E \ \Delta g^0 - \Delta f^0) \left\{ a_{k+sn} - \frac{|b_{k+sn}|^2}{\lambda + r_k} a_k^{(n)} \right\}$$

$$- (E \ \Delta g^1 - \Delta f^1) \left\{ b_{k+sn} - \frac{|b_{k+sn}|^2}{\lambda + r_k} b_k^{(n)} \right\}$$

$$+ (m_k b_k)^{(n)} \frac{|b_{k+sn}|^2}{\lambda + r_k} - m_{k+sn} b_{k+sn} \ . \tag{3.44}$$

Further, if $f \in C^4$ we have

$$m_k = \Delta f^2 a_k - \Delta f^3 b_k + f_k^{(4)} b_k \tag{3.45}$$

with

$$\Delta f^2 = f^{(2)}(1) - f^{(2)}(0) \ ,$$

$$\Delta f^3 = f^{(3)}(1) - f^{(3)}(0) \ ,$$

$$f_k^{(4)} = \int_0^1 \exp \ (2\pi i k t) f^{(4)}(t) dt \ .$$

The last term on the right of (3.44) can then be rewritten as

$$\Delta f^2 \left\{ (a_k b_k)^{(n)} \frac{|b_{k+sn}|^2}{\lambda + r_k} - a_{k+sn} b_{k+sn} \right\}$$

$$- \Delta f^3 \left\{ (b_k^2)^{(n)} \frac{|b_{k+sn}|^2}{\lambda + r_k} - b_{k+sn}^2 \right\}$$

$$+ \left\{ (f_k^{(4)} b_k^2)^{(n)} \frac{|b_{k+sn}|^2}{\lambda + r_k} - f_{k+2n}^{(4)} b_{k+sn}^2 \right\} \ . \tag{3.46}$$

Let

$$A_0(t) = -\sum_s \sum_{k=1}^{n-1} \left\{ (b_k^2)^{(n)} \frac{|b_{k+sn}|^2}{\lambda+r_k} - b_{k+sn}^2 \right\} \exp(-2\pi i(k+sn)t) ,$$

$$A_1(t) = -\sum_s \sum_{k=1}^{n-1} \left\{ (a_k b_k)^{(n)} \frac{|b_{k+sn}|^2}{\lambda+r_k} - a_{k+sn}b_{k+sn} \right\} \exp(-2\pi i(k+sn)t) ,$$

$$A_2(t) = \sum_s \sum_{k=1}^{n-1} \left\{ b_{k+sn} - \frac{|b_{k+sn}|^2}{\lambda+r_k} b_k^{(n)} \right\} \exp(-2\pi i(k+sn)t) ,$$

$$A_3(t) = \sum_s \sum_{k=1}^{n-1} \left\{ a_{k+sn} - \frac{|b_{k+sn}|^2}{\lambda+r_k} a_k^{(n)} \right\} \exp(-2\pi i(k+sn)t) .$$

Set

$$B_j(t) = \lambda \sum_{k\neq 0} \frac{(2\pi i k)^j}{\lambda(2\pi k)^4+1} \exp(-2\pi i k t), \quad j=0,1,2,3 .$$

__Lemma 4.__ *If* $\lambda^3 n^8 \to \infty$, $\lambda \to 0$ *as* $n \to \infty$ *then*

$$\int_0^1 |A_j(t)-B_j(t)|^2 \, dt = o\!\left(\lambda^{\frac{7-2j}{4}}\right), \qquad j=0,1,2,3 . \qquad (3.47)$$

Also $\int_0^1 |B_j(t)|^2 \, dt$ *tends to zero at the rate of* $\lambda^{\frac{7-2j}{4}}$, $j=0,1,2,3$.

The estimates required for this lemma parallel those used to obtain (3.29) and (3.31).

We wish to get more convenient representations or estimates of the $B_j(t)$'s. A contour integration shows that

$$C_0(t) = \frac{1}{2\pi} \int \frac{e^{itx}}{1+x^4} \, dx = \frac{1}{2\sqrt{2}} e^{-|t|2^{-\frac{1}{2}}} \left(\cos(t2^{-\frac{1}{2}}) + \sin(|t|2^{-\frac{1}{2}})\right) .$$

Successive differentiation then indicates that

$$C_1(t) = \frac{1}{2\pi} \int \frac{e^{itx} ix}{1+x^4} \, dx = -\frac{1}{2} e^{-|t|2^{-\frac{1}{2}}} \sin(t2^{-\frac{1}{2}}) ,$$

$$C_2(t) = \frac{1}{2\pi} \int \frac{e^{itx}(ix)^2}{1+x^4} \, dx = \frac{1}{2\sqrt{2}} e^{-|t|2^{-\frac{1}{2}}} \left(\sin(|t|2^{-\frac{1}{2}}) - \cos(t2^{-\frac{1}{2}})\right) ,$$

$$C_3(t) = \frac{1}{2\pi} \int \frac{e^{itx}(ix)^3}{1+x^4} \, dx = \frac{1}{2} \operatorname{sgn} t \; e^{-|t|2^{-\frac{1}{2}}} \cos(t2^{-\frac{1}{2}}) .$$

An application of the Poisson summation formula tells us that

$$B_j(t) = \lambda^{\frac{3-j}{4}} \sum_k C_j((k-t)\lambda^{\cdot}) . \tag{3.48}$$

Only the terms in the sum (3.48) corresponding to $k = 0$, $k = 1$ need to be considered since the sum of the remaining terms die off at the rate $e^{-\alpha\lambda^{-\frac{1}{4}}}$ with α a positive constant. Notice that the formulas for the $C_j(t)$ above imply that

$$C_1 = C_3 = \frac{1}{2\sqrt{2}} .$$

<u>Lemma 5.</u> *Assume that* $f \in C^4$. *Then if* $\Delta f^2 \neq 0$

$$E \; \Delta g^0 - \Delta f^0 \cong - \lambda^{1/2} \Delta f^2 \tag{3.49}$$

while if $\Delta f^2 = 0$

$$E \, \Delta g^0 - \Delta f^0 \cong 2\sqrt{2} \, \lambda^{3/4} \, \frac{1}{2} \, \{f^{(3)}(0) + f^{(3)}(1)\}. \tag{3.50}$$

$If \; f^{(2)}(0) + f^{(2)}(1) \neq 0 \;\; we \; have$

$$E \, \Delta g^1 - \Delta f^1 \cong - \, 2\sqrt{2} \, \lambda^{1/4} \, \frac{1}{2} \, \{f^{(2)}(0) + f^{(2)}(1)\} \tag{3.51}$$

$and \; if \; f^{(2)}(0) + f^{(2)}(1) = 0$

$$E \, \Delta g^1 - \Delta f^1 \cong \Delta f^3 \lambda^{1/2} \tag{3.52}$$

$as \;\; \lambda = \lambda(n) \to 0.$

The asymptotic relations (3.49) and (3.50) follow from (3.40), (3.43) and (3.45). Formula (3.51) is a consequence of (3.41) and (3.42). If $f^{(2)}(0) + f^{(2)}(1) = 0$, since $\sum \mathrm{Re} \, m_k = \frac{1}{2} \, (f^{(2)}(0) + f^{(2)}(1))$ one can see that

$$\sum \frac{\mathrm{Re} \, m_k}{1+\lambda(2\pi k)^4} = - \sum \frac{\lambda(2\pi k)^4 \, \mathrm{Re} \, m_k}{1+\lambda(2\pi k)^4} \, . \tag{3.53}$$

However by (3.45)

$$\mathrm{Re} \, m_k = \frac{\Delta f^3}{(2\pi k)^2} - \frac{1}{(2\pi k)^2} \int \frac{1}{2} \, (f^{(4)}(x) + f^{(4)}(-x)) \cos 2\pi kx \, dx \tag{3.54}$$

This implies (3.52).

<u>Lemma 6.</u> $Let \;\; f \in C^4. \;\; If \;\; f^{(2)}(0) \neq 0, \; f^{(2)}(1) = 0 \;\; then$

$$E\ g(t)-f(t) = f^{(2)}(0)\ \lambda^{\frac{1}{2}}e^{-t2^{-\frac{1}{2}}\lambda^{-\frac{1}{4}}}\ [\sin(t2^{-\frac{1}{2}}\lambda^{-\frac{1}{4}}) - \cos(t2^{-\frac{1}{2}}\lambda^{-\frac{1}{4}})]$$

$$+\ e(t)\ , \qquad (3.55)$$

$0 < t < 1$, *where the error term* $e(t)$ *is such that*

$$\int e(t)^2\ dt = o\left(\int [E\ g(t)-f(t)]^2\ dt\right). \qquad (3.56)$$

If $f^{(2)}(0) = f^{(2)}(1) = 0$, $f^{(3)}(0) \neq 0$, $f^{(3)}(1) = 0$, *we have*

$$E\ g(t)-f(t) = f^{(3)}(0)\lambda^{3/4}\ \sqrt{2}\ e^{-t2^{-\frac{1}{2}}\lambda^{-\frac{1}{4}}}\ \cos(t2^{-\frac{1}{2}}\lambda^{-\frac{1}{4}}) + e(t) \qquad (3.57)$$

$0 < t < 1$, *where the error term again satisfies* (3.56). *The approximations appropriate for the cases* $f^{(2)}(0) = 0$, $f^{(2)}(1) \neq 0$ *and* $f^{(2)}(0) = f^{(2)}(1) = 0$, $f^{(3)}(0) = 0$, $f^{(3)}(1) \neq 0$ *are obtained by replacing* t *by* $1-t$ *in the main expressions on the right of* (3.55) *and* (3.57) *respectively.*

We next consider the variance and bias of the derivative g' of the smoothing spline. Theorems 2 and 3 follow from the previous analysis of g, after noting that the Fourier coefficients of g' are

$$g_0' = \Delta g^0 \qquad (3.58)$$

$$g_k' = a_k \Delta g^1 - a_k h_k, \qquad k \neq 0 . \qquad (3.59)$$

We first consider the integrated squared variance

$$V = \sum \sigma^2(g_k') .$$

From (3.26),

$$\sigma^2(g_0) \cong \frac{\sigma^2}{n} c_2 c_1^{-2} \lambda^{-1/4} .$$

As in (3.16)

$$a_{k+sn}\Delta g^{\prime} - a_{k+sn}h_{k+sn} = a_{k+sn}\Delta g^1 \left(1 - \frac{1}{\lambda+r_k} b_{k+sn}b_k^{(n)}\right)$$

$$+ a_{k+sn}a_k^{(n)}\Delta g^0 - \frac{a_{k+sn}b_{k+sn}}{\lambda+r_k} \frac{\hat{y}_k}{\sqrt{n}} \tag{3.60}$$

Estimates similar to those used in the analysis of the smoothing spline show that the contribution to the variance from the first term is of order $\lambda^{-\frac{1}{2}}n^{-1}$. The second term gives a contribution of order $\lambda^{-\frac{1}{4}}n^{-1}$; the third term dominates, giving a total contribution to V

$$\cong \frac{\sigma^2}{n} \sum \frac{|2\pi i k|^2}{[\lambda(2\pi i k)^4+1]^2}$$

$$\cong \frac{\sigma^2}{n} \lambda^{-3/4} \int_{-\infty}^{\infty} \frac{(2\pi x)^2}{((2\pi x)^4+1)^2} dx . \tag{3.61}$$

Next, the bias:

$$E g_{k+sn}^{\prime} - f_{k+sn}^{\prime} = a_{k+sn}(E \Delta g^1 - \Delta f^1)$$

$$- a_{k+sn}(E h_{k+sn} - m_{k+sn}) \tag{3.62}$$

which, as in (3.44)

$$= (E \, \Delta g^0 - \Delta f^0) \, \frac{b_{k+sn} a_{k+sn} a_k^{(n)}}{\lambda + r_k}$$

$$+ (E \, \Delta g^1 - \Delta f^1) \left[a_{k+sn} - \frac{b_k^{(n)} a_k^{(n)} b_{k+sn}}{\lambda + r_k} \right]$$

$$- a_k \left[\frac{(m_k b_k)^{(n)} b_{k+sn}}{\lambda + r_k} - m_{k+sn} \right] . \tag{3.63}$$

Making approximations as in the analysis of the spline function itself,

$$E \, g'(t) - f'(t) \cong (E \, \Delta g^0 - \Delta f^0) + (E \, \Delta g^0 - \Delta f^0) \, \lambda^{-1} \, B_0(t)$$

$$+ (E \, \Delta g^1 - \Delta f^1) \, B_3(t) + \Delta f^2 B_2(t) - \Delta f^3 B_1(t) .$$

Using the Poisson-summation approximation and Lemma 5 if $f^{(2)}(0) \neq 0$, $f^{(2)}(1) = 0$,

$$E \, g'(t) - f'(t) \cong f^{(2)}(0) \, 2^{\frac{1}{2}} \, \lambda^{\frac{1}{4}} \, e^{-u} \cos u$$

where $u = 2^{-\frac{1}{2}} \, \lambda^{-\frac{1}{4}} t$. If $f^{(2)}(0) = f^{(2)}(1) = 0$, and $f^{(3)}(0) \neq 0$, $f^{(3)}(1) = 0$

$$E \, g'(t) - f'(t) \cong - f^{(3)}(0) \, \lambda^{\frac{1}{2}} \, e^{-u} \, (\sin u + \cos u) .$$

Note that the approximate (in an L_2 sense) bias of the derivative is the derivative of the approximate bias (Lemma 6).

4. Deconvolution

We now sketch the development of the deconvolution results. Since this parallels closely the derivations of Section 3 the presentation will be somewhat sketchier. As before let g have Fourier coefficients

$$g_k = \Delta g^0 a_k - \Delta g^1 b_k + h_k b_k \qquad k \neq 0 \tag{4.1}$$

and let

$$G_k = w_k \, g_k$$

$$A_k = w_k \, a_k$$

$$B_k = w_k \, b_k$$

$$H_k = w_k \, b_k \, h_k$$

and define y_j as in Section 3. Then (1.7) may be written as

$$\left| \frac{\hat{y}_0}{\sqrt{n}} - G_0 - \tilde{G}_0^{(n)} \right|^2 + \sum_{k=1}^{n-1} \left| \frac{\hat{y}_j}{\sqrt{n}} - G_j^{(n)} \right|^2$$

$$+ \lambda \left[(\Delta g^1)^2 + \sum_{j=1}^{n-1} \sum_s |h_{j+sn}|^2 \right]. \tag{4.2}$$

Minimizing the 0th term gives $h_{sn} = 0$, $s \neq 0$, and $G_0 + \tilde{G}_0^{(n)} = \hat{y}_0/\sqrt{n}$.

As in the analysis of Section 3, we first fix Δg^0 and Δg^1 and minimize with respect to the h_j's. If

$$\hat{z}_j = \frac{\hat{y}_j}{\sqrt{n}} - \Delta g^0 A_j^{(n)} + \Delta g^1 B_j^{(n)} \ .$$

Then (4.2) becomes

$$\sum' \ |\hat{z}_j - H_j^{(n)}|^2 + \lambda \left[(\Delta g^1)^2 + \sum_k' \sum_s |H_{k+sn}|^2 \ |B_{k+sn}|^{-2} \right] \ . \qquad (4.3)$$

The minimizing coefficients can be calculated to be

$$h_{j+sn} = \overline{B}_{j+sn} \frac{\hat{z}_j}{\lambda + p_j} \qquad (4.4)$$

where $p_j = \sum\limits_{s=-\infty}^{\infty} |B_{j+sn}|^2$. Now to calculate the minimizing Δg^0 and Δg^1, this solution is substituted back into (4.3) to give

$$\lambda \sum' \ |\hat{z}_j|^2 \ (\lambda + p_j)^{-1} + \lambda (\Delta g^1)^2 \ . \qquad (4.5)$$

Minimizing this with respect to Δg^0 and Δg^1 amounts to solving two linear equations in two unknowns, and it may be seen that the solution is approximately

$$\Delta g^0 \cong \left\{ \mathrm{Re} \sum' \frac{\overline{\hat{y}}_j}{\sqrt{n}} A_j^{(n)} \ (\lambda + p_j)^{-1} \right\} \left\{ \sum' \ |A_j^{(n)}|^2 \ (\lambda + p_j)^{-1} \right\}^{-1} \ , \qquad (4.6)$$

$$\Delta g^1 \cong - \left\{ \Delta f^1 + \mathrm{Re} \sum' \frac{\overline{\hat{y}}_j}{\sqrt{n}} B_j^{(n)} \ (\lambda + p_j)^{-1} \right\} \left\{ 1 + \sum |B_j^{(n)}|^2 \ (\lambda + p_j)^{-1} \right\}^{-1} \ . $$

$$(4.7)$$

We next consider the integrated squared variance, which is the sum of the variance of the Fourier coefficients of g. Now, from above,

$$g_{j+sn} = \Delta g^0 \left[a_{j+sn} - \frac{|b_{j+sn}|^2 \overline{w}_{j+sn} A_j^{(n)}}{\lambda + p_j} \right]$$

$$+ \Delta g^1 \left[b_{j+sn} - \frac{|b_{j+sn}|^2 \overline{w}_{j+sn} B_j^{(n)}}{\lambda + p_j} \right]$$

$$+ \frac{|B_{j+sn}|^2}{\lambda + p_j} \frac{\hat{y}_j}{\sqrt{n}} . \tag{4.8}$$

Via approximations similar to those in Section 3, it may be seen that the first two terms contribute a net variance of order $n^{-1}\lambda^{-2\beta/(2\beta+4)}$ whereas the third term contributes the dominating variance, which is of order $n^{-1}\lambda^{-(2\beta+1)/(2\beta+4)}$.

If we write the Fourier coefficients of f as

$$f_k = \Delta f^0 a_k - \Delta f^1 b_k + m_k \tag{4.9}$$

and take expectations in (4.8), the bias of the $(j+sn)^{th}$ Fourier coefficient may be expressed as

$$E\, g_{k+sn} - f_{k+sn} = (E\,\Delta g^0 - \Delta f^0) \left[a_{k+sn} - \frac{|b_{k+sn}|^2 \overline{w}_{k+sn} A_k^{(n)}}{\lambda + p_k} \right]$$

$$- (E\,\Delta g^1 - \Delta f^1) \left[b_{k+sn} - \frac{|b_{k+sn}|^2 \overline{w}_{k+sn} B_k^{(n)}}{\lambda + p_k} \right]$$

$$+ \frac{|b_{k+sn}|^2 \overline{w}_{k+sn} M_k^{(n)}}{\lambda + p_k} - m_{k+sn} b_{k+sn} . \tag{4.10}$$

As in section 3 for $|k| \leq n/2$, $k \neq 0$

$$E\, g_k - f_k \cong (E\,\Delta g^0 - \Delta f^0)\, \frac{\lambda a_k}{\lambda + |B_k|^2}$$

$$- (E\,\Delta g^1 - \Delta f^1)\, \frac{\lambda b_k}{\lambda + |B_k|^2}$$

$$+ \Delta f^2\, \frac{\lambda a_k b_k}{\lambda + |B_k|^2}$$

$$- \Delta f^3\, \frac{\lambda b_k^2}{\lambda + |B_k|^2}$$

$$+ \frac{\lambda f_k^{(4)} b_k^2}{\lambda + |B_k|^2}\, . \qquad (4.11)$$

If we let

$$D_j(t) = \lambda \sum_k{}' \frac{k^{4-j}}{\lambda + |B_k|^2}\, \exp(-2\pi i k t) \qquad j = 0,1,2,3 \qquad (4.12)$$

(note that $\|D_j\|^2 \sim \lambda^{(7-2j)/(4+2\beta)}$) then

$$E\, g(t) - f(t) \cong (E\,\Delta g^0 - \Delta f^0) D_3(t)\ -\ (E\,\Delta g^1 - \Delta f^1) D_2(t)$$

$$+ \Delta f^2 D_1(t)\ -\ \Delta f^3 D_0(t)$$

$$+ \lambda \sum \frac{f_k^{(4)}\, b_k^2}{\lambda + |B_k|^2}\, \exp(-2\pi i k t)\ . \qquad (4.13)$$

The function $D_j(t)$ play the role of the functions $B_j(t)$ of section 3. Although their exact analytical forms depend on w, they are, like the B_j's, successively odd and even, and are increasingly peaked near 0 and 1 as $\lambda \to 0$.

We now consider the individual terms in (4.13). From (4.6) it follows that

$$E \Delta g^0 - \Delta f^0 = \frac{\sum' m_k B_k \overline{A}_k (\lambda + p_k)^{-1}}{\sum' |A_k|^2 (\lambda + p_k)^{-1}} .$$

The denominator can be estimated to be $\sim \lambda^{3/(2\beta+4)}$. If $\Delta f^2 \neq 0$, the numerator is

$$\cong \Delta f^2 \sum |B_k|^2 (\lambda + p_k)^{-1} \sim \lambda^{-1/(2\beta+4)} .$$

In combination with D_3 this gives a net contribution to the integrated squared bias which is $\sim \lambda^{5/(2\beta+4)}$. If $\Delta f^2 = 0$ the numerator is $\cong (f^{(3)}(1) + f^{(3)}(0))/2$, giving a net contribution of order $\lambda^{7/(2\beta+4)}$. If $f^{(k)}(0) = f^{(k)}(1) = 0$ $k = 2,3$ the net contribution is $0(\lambda^2)$.

Next,

$$E \Delta g^1 - \Delta f^1 \cong \frac{\Delta f^1 + \sum' m_j |B_j|^2 (\lambda + p_k)^{-1}}{1 + \sum' |B_j|^2 (\lambda + p_k)^{-1}} .$$

The denominator is $\sim \lambda^{-1/(2\beta+4)}$ and if $f^{(2)}(1)$ or $f^{(2)}(0) \neq 0$ the numerator is $\cong (f^{(2)}(1) + f^{(2)}(0))/2$. This gives a net contribution to

the integrated squared bias of order $\lambda^{5/(2\beta+4)}$. If both second derivatives are zero the numerator is

$$\cong \lambda\Delta f^3 \sum \frac{b_k}{\lambda+|B_k|^2} \sim \lambda^{1/(2\beta+4)}$$

giving a net contribution of order $\lambda^{7/(2\beta+4)}$. If both second and third derivatives vanish at 1 and 0 the net contribution is $O(\lambda^2)$.

The last term in (4.11) can be estimated and makes a contribution to the integrated squared bias of order λ^2.

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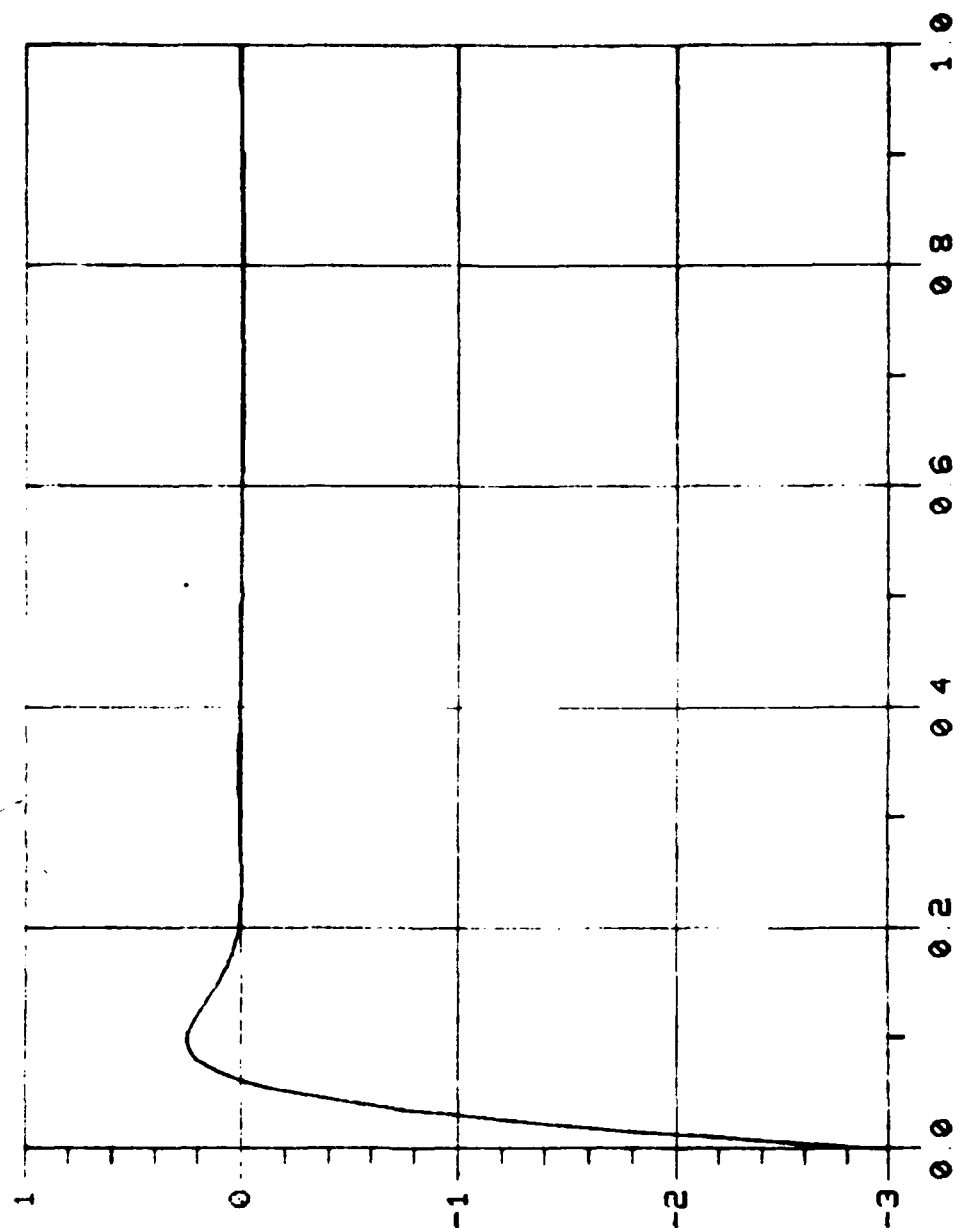Whittaker, E. (1923). On a new method of graduation. Proc. Edinburgh Math. Soc., 41, 63-75.

Figure 1

LAMBDA = 0 104E-35

BIAS OF FUNCTION

$\cos(2\pi t) + 4 \cos \pi t$

0 06

0 04

0 02

0 00

-0 02

0 0   0 2   0 4   0 6   0 8   1 0
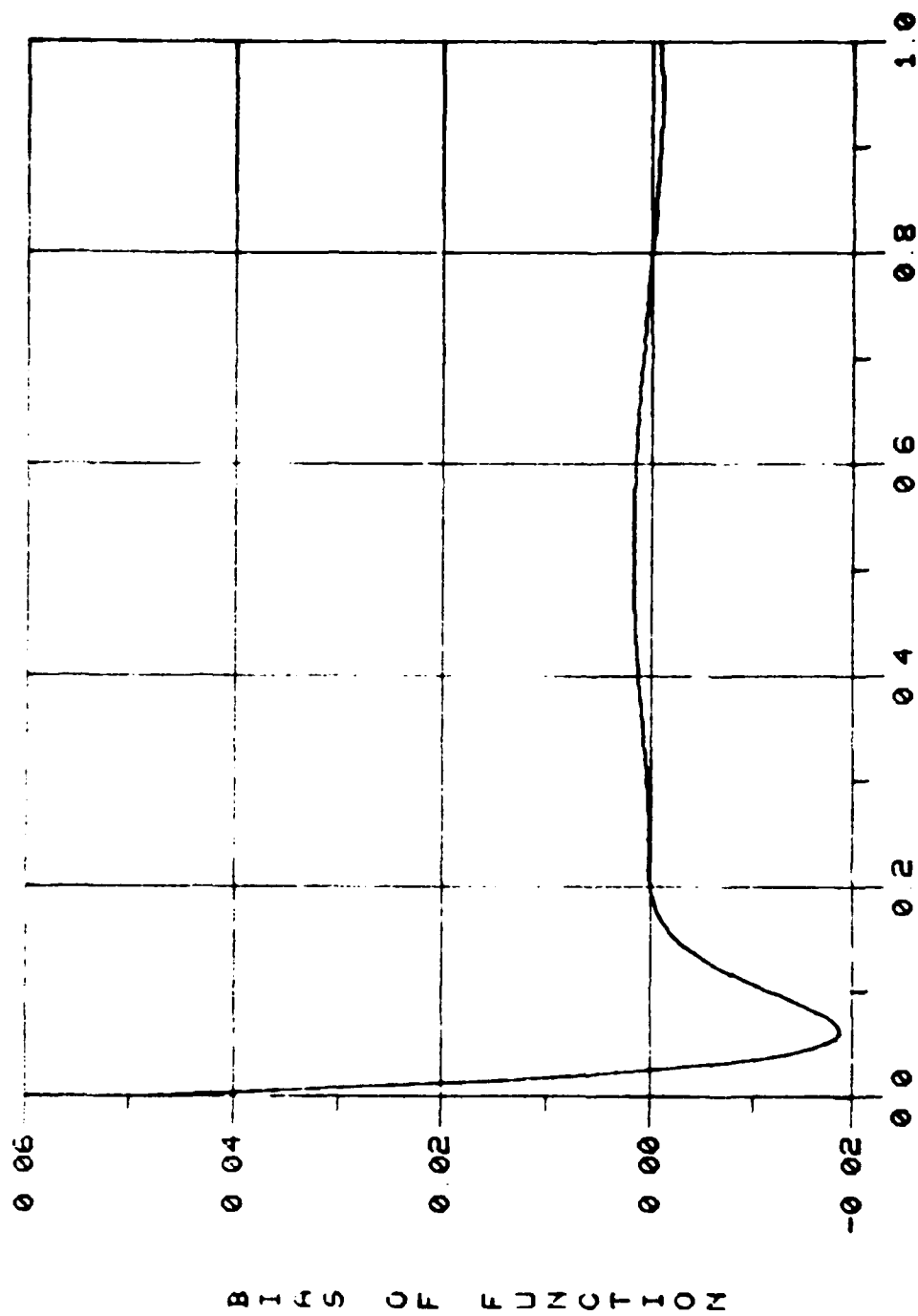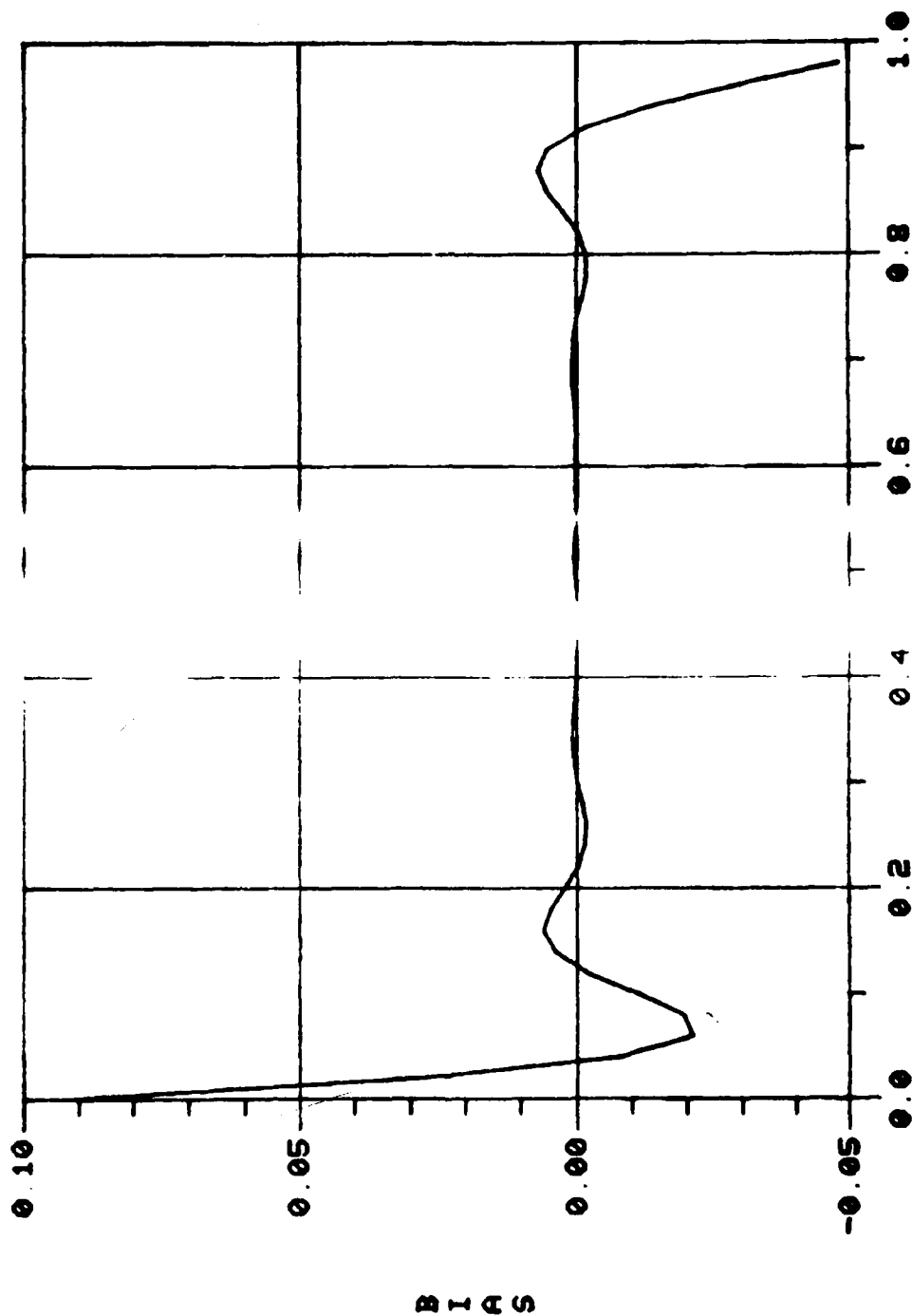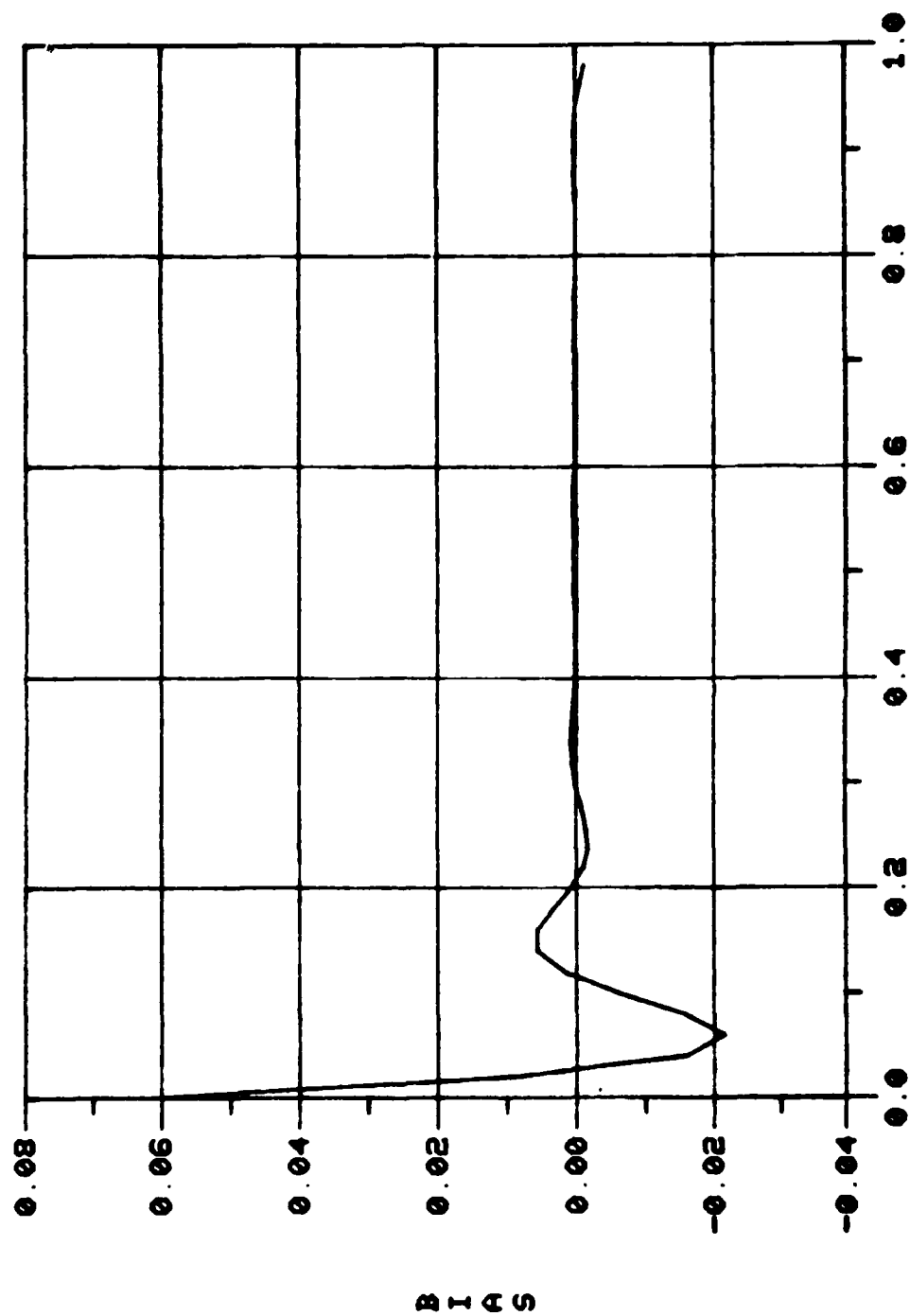
Figure 2

LAMBDA = 0.203E-05

BIAS OF DERIVATIVE

Figure 3

LAMBI... 3 30E-07

Figure 4

LAMBDA = 0 100E-07

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